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Journal of Molecular Structure 595 (2001) 15–20

Journal of
MOLECULAR
STRUCTURE

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The structure of 1-phenyl-3-methyl-4-benzoylpyrazol-2-in-5-selenone and its derivatives

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Received 23 October 2000; revised 2 January 2001; accepted 2 January 2001

Abstract

It is shown that 1-phenyl-3-methyl-4-benzoylpyrazol-2-in-5-selenone exists in a SeH-tautomeric form in the solid phase. Crystal and molecular structure of bis(1-phenyl-3-methyl-4-benzoylpyrazolyl-5)selenide as a supplementary product of the synthesis of selenopyrazolone and di(1-phenyl-3-methyl-4-benzoylselenopyrazolyl-5)diselenide as the product of oxidation of the latter were characterised by X-ray single crystal diffraction.

Keywords: Selenopyrazolones and pyrazolones; Tautomerism; X-ray single crystal diffraction

1. Introduction

Unlike a great number of publications devoted to synthesis, structure and reactivity of pyrazol-2-in-5-ones, widely used in pharmacology, dyeing industry, and in metal extracting processes, chemistry of their chalcogen containing analogues is hardly explored. Although the first representatives of thio and selenopyrazolones were synthesised by German chemists as far back as in the beginning of the century [1,2], their structure remained unknown until recently. There were only few publications concerning tautomerism, acid–base and other properties of chalcogenopyrazolones [3–8]. Judging by the results of our theoretical works [9–11], thio and selenopyrazolones must perceptibly differ from their oxygen analogues by the stability of their tautomeric forms and inclination to the processes of proton and electron transfer, etc. Experimental reliability of the theoretical predictions was recently confirmed by us for thiopyrazolones [12,13].

The aim of the present work was to study the structure of 1-phenyl-3-methyl-4-benzoylpyrazol-2-in-5-selenone (**I**), hereafter referred to as selenopyrazolone, in comparison with the structure of its oxo and thio analogues studied earlier [12,14–18]. First of all, we were interested in the stability of the tautomeric forms of selenopyrazolone (**I**) and the possibility of

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0022-2860/01/$ - see front matter
PII: S0022-2860(01)00478-1